Tikrit Journal of Pure Science Vol. 31 (4) 2026

DOI:https://doi.org/10.25130/tjps.v31i4.2030

IRAQI Academic Scientific Journals

Tikrit Journal of Pure Science

ISSN: 1813 – 1662 (Print) --- E-ISSN: 2415 – 1726 (Online)

Journal Homepage: https://tjpsj.org/

Theoretical Study of Carrier Concentration Impact on the Photocurrent and Efficiency of RuTH–TiO_2 DSSCs

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Received: 8 May. 2025 **Received in revised forum:** 12 Jul. 2025 **Accepted:** 16 Jul. 2025

Final Proofreading: 27 Jul. 2025 **Available online:** 25 Aug. 2026

ABSTRACT

In this work, we study and calculate the efficiency of RuTH dye-contact TiO_2 semiconductor-based dye-sensitized solar cells (DSSCs) using quantum charge transport. We studied and evaluated the impact of flow current density, based on interface reorganization energy, force coupling, atomic density, effective path length and the concentration and polarity of both RuTH and TiO_2 dyes, on the charge-transport process. We discussed and analyzed the influence of strong coupling and concentration on flow current density in RuTH-TiO_2 devices, as reflected in the electronic transfer results. The results show that flow current density is strongly affected by concentration and strength coupling, which determine the efficiency of RuTH-TiO_2 devices. The efficiency, influenced by the increased carrier concentration of TiO_2, plays a significant role in the increased flow of current in the charge transport reaction and limits the electrical properties of RuTH-TiO_2 devices. Specifically, the strength of the coupling between the RuTH dye and TiO_2 affects electron transport. It plays a key role in modulating current density and efficiency; stronger coupling increases electron transport, and vice versa. Additionally, increasing the concentration from (2×10^{18} cm^{-3}) to (4×10^{18} cm^{-3}) is favorable and increases efficiency from (4.543 %) to (9.227 %); this suggests that RuTH dye is a suitable contact for TiO_2-based DSSC devices.

Keywords: Concentration, DSSC, Efficiency, Ruthenium dipyridine, TiO_2.

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Tikrit Journal of Pure Science Vol. 31 (4) 2026
DOI:https://doi.org/10.25130/tjps.v31i4.2030

دراسة نظرية لتأثير تركيز الناقلات على التيار الضوئي وكفاءة خلايا RuTH–TiO_2 DSSCs

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الملخص

في هذا العمل، تم دراسة وحساب كفاءة أشباه الموصلات TiO_2 الملامسة لصبغة RuTH في الخلايا الشمسية الحساسة للصبغة DSSCs باستخدام نقل الشحنة الكمي. تمت دراسة وتقييم تأثير كثافة تيار التدفق بناءً على طاقة إعادة تنظيم الواجهة، واقتران القوة، والكثافة الذرية، وطول المسار الفعال، والتركيز والقطبية لكل من صبغات RuTH وغشاء TiO_2على عملية نقل الشحنة. تمت مناقشة وتحليل تأثير اقتران القوة والتركيز على سلوك كثافة تيار التدفق في أجهزةRuTH-TiO_2 ، والذي ينعكس في نتائج النقل الإلكتروني. تكشف النتائج أن سلوك كثافة تيار التدفق تأثر بشدة بالتركيز واقتران القوة، مما يحدد كفاءة صبغة غشاء RuTH-TiO_2، وتلعب الكفاءة، المتأثرة بزيادة تركيز الناقل لـTiO_2، دورًا مهمًا في زيادة تيار التدفق لتفاعل نقل الشحنة وتحد من الخصائص الكهربائية لصبغة غشاء RuTH-TiO_2. على وجه التحديد، يؤثر اقتران القوة المتداخل بين صبغة RuTH و TiO_2 على تفاعل النقل الإلكتروني. لقد لعب النقل الالكتروني دورًا رئيسيًا في تعديل كثافة تيار التدفق المتزايد والكفاءة، مع زيادة في قوة الاقتران تتوافق مع نقل الإلكترون، والعكس صحيح. بالإضافة إلى ذلك، فإن الزيادة في التركيز الناقل من (2×10^{18} cm^{-3}) إلى (4×10^{18} cm^{-3}) مواتية وتزيد من الكفاءة من (4.543 %) إلى (9.227 %)، وهذا يشير إلى أن صبغة RuTH هي عامل اتصال مناسبة لخلايا DSSCs القائمة على TiO_2 .

INTRODUCTION

Global population growth has increased the demand for renewable and clean energy for sustainable development in various areas of the world. Recently, statistics have indicated that many countries have relied on limited and non-renewable resources, which has caused more global environmental pollution and global warming [(1)]. Dye contacts have been used with semiconductor interfaces in major mainstream devices, solar cells, and electronic devices [(2)]. Dye-sensitized solar cells (DSSCs) are the main types of third-generation solar cell devices and are interesting for their fundamental technologies that convert photon light into electricity at low cost as a result of low-cost manufacturing and optical properties [(3)]. Semiconductors have a wide range of properties between insulation and conduction as the basis for solar cells, integrated circuit devices, and are essential for many technological applications [(4)]. The main fundamental interactions at work in dual photovoltaic cells depend on the photoinduced charge transfer interaction through the interfaces of the contact materials in the devices and the materials in the electrochemical devices, and it requires the reconfiguration of energy levels to become locked with each other [(5, 6)]. In recent years, titanium dioxide (TiO_2) has received more attention as a vital element towards primary doping to achieve exceptional physical properties; absorption, stability, high mobility, wide band gap and adaptability to different temperatures in a wide range of optoelectronic applications [(7)]. Charge transfer across the interface of two materials occurs when one material is attached to another. This occurs when the work function of the acceptor material is higher than that of the donor material. As a result, charges move from the donor to the acceptor until their energy levels align with each other [(8)]. The charge transfer at the RuTH Dye - TiO_2 interface are illustrated in Figure (1) [(9)].

DOI:https://doi.org/10.25130/tjps.v31i4.2030

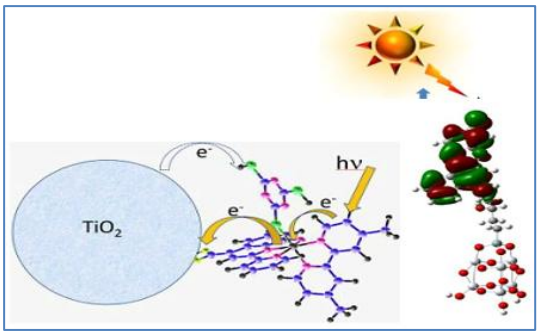


Fig.1: Charge transfer at RuTH –TiO_2 contact [9]

In this paper, increasing carrier concentration by light absorption effect on the charge transfer reaction across the interface between the ruthenium dye RuTh contact with TiO_2 semiconductor-based DSSC has been investigated and studies using simple charge transfer reaction.

THEORY

The flow current $I_F(E)$ for charge transfer from RuTh dye to TiO_2 is given by [10].

$$I_F(E) = \sum qF(E)T_F(E) \quad \dots (1)$$

Where q is charge transfer, $F(E)$ is the distribution density function in donor–acceptor system, $T_F(E)$ is the charge transfer coefficient and written by:

$$T_F(E) = \frac{4\pi^2}{h} |\langle S_C \rangle|^2 \rho_f(E) \quad \dots (2)$$

Where h is Planck constant, $\langle S_C \rangle$ is overlap coupling constant and $\rho_f(E)$ is the density in device system and gives by [11]:

$$\rho_f(E) = \frac{l_f \rho_S}{(\frac{6}{\pi})^{1/3}} \quad \dots (3)$$

Where ρ_S and l_f are charge density in TiO_2 and length path in semiconductor. The flow charge density ρ_S in semiconductor is [12]:

$$\rho_S = \langle \hat{\boldsymbol{\rho}}_{ss} \rangle \rho_N(E) d_S^{-2/3} \quad \dots (4)$$

Where $\langle \hat{\boldsymbol{\rho}}_{ss} \rangle$ is the density of state in system, $\rho_N(E)$ is the density of state in dye and d_s is the atomic density of semiconductor. The density of state in system $\langle \hat{\boldsymbol{\rho}}_{ss} \rangle$ is given by[13]:

$$\langle \hat{\boldsymbol{\rho}}_{ss} \rangle = \frac{1}{\sqrt{4\pi \lambda_S^N k_B T}} e^{-\frac{(\Delta V^0 + \lambda_S^N)^2}{4\lambda_S^N k_B T}} \quad \dots (5)$$

Where ΔV^0 is the driving free energy, λ_S^N is the reorganization energy, k_B is Boltzman constant, and T is room temperature. The reorganization energy λ_S^N (eV) in donor–acceptor-solvent system is [14]:

$$\lambda_S^N \text{ (eV)} = \frac{e^2}{8D\pi\varepsilon_\circ}\left[\frac{1}{n^2} - \frac{1}{\varepsilon}\right] + \frac{e^2}{16R\pi\varepsilon_\circ}\frac{1}{2R}\left[\frac{\varepsilon_S^2 - \varepsilon^2}{\varepsilon_S^2 + \varepsilon^2}\frac{1}{\varepsilon^2} - \frac{n_S^2 - n^2}{n_S^2 + n^2}\frac{1}{n^2}\right] \quad \dots (6)$$

where e and $\varepsilon_\circ$ are charge and permittivity. The R and D are the distance between molecule and semiconductor and radius of dye, ε and n are dielectric constant and refractive index of solvent, ε_S and n_S are dielectric constant and refractive index of semiconductor. The radius D is [15]:

$$D = (\frac{3}{4\pi})^{\frac{1}{3}}(\frac{m}{N\rho})^{\frac{1}{3}} \quad \dots (7)$$

where m, N, and ρ are molecular weight, Avogadro number and the density. Inserting Eq. (5) in Eq.(4) to obtained the flow charge density:

$$\rho_S = \frac{\rho_N(E) d_S^{-2/3}}{\sqrt{4\pi \lambda_S^N k_B T}} e^{-\frac{(\Delta V^0 + \lambda_S^N)^2}{4\lambda_S^N k_B T}} \quad \dots (8)$$

Inserting Eqs.(8) and (5) in Eq.(2) to give:

$$T_F(E) = \frac{4\pi^2}{h} |\langle S_C \rangle|^2 \frac{l_f}{(\frac{6}{\pi})^{1/3}} \frac{\rho_N(E) d_S^{-2/3}}{\sqrt{4\pi \lambda_S^N k_B T}} e^{-\frac{(\Delta V^0 + \lambda_S^N)^2}{4\lambda_S^N k_B T}} \quad \dots (9)$$

The Eq. (9) together Eq. (1) and assume $F(E) = F_D(E) - F_A(E)$ for continuum system and integrated over energy E to obtain. The flow current $I_F(E)$ in Eq.(1) for charge transfer together Eq. (10) from RuTh dye to TiO_2 becomes:

$$I_F(E) = \frac{4q\pi^2}{h} \sum F(E) |\langle S_C \rangle|^2 \frac{l_f}{(\frac{6}{\pi})^{1/3}} \frac{\rho_N(E) d_S^{-2/3}}{\sqrt{4\pi \lambda_S^N k_B T}} e^{-\frac{(\Delta V^0 + \lambda_S^N)^2}{4\lambda_S^N k_B T}} \quad \dots (10)$$

The summation integral in Eq. (10) is given [16]:

$$\sum F(E)\rho_N(E) = [C] \quad \dots (11)$$

Where $[C]$ is carrier concentration in (states/ cm^3). The Eq. (10) together Eq. (11) to yield:

$$I_F(E) = \frac{4q\pi^2}{h} [C] |\langle S_C \rangle|^2 \frac{l_f}{(\frac{6}{\pi})^{1/3}} \frac{d_S^{-2/3}}{\sqrt{4\pi \lambda_S^N k_B T}} e^{-\frac{(\Delta V^0 + \lambda_S^N)^2}{4\lambda_S^N k_B T}} \quad \dots (12)$$

The flow current density $J_F(E)$ in Eq. (12) for charge transfers function of area of solar cells A is:

$$J_F(E) = \frac{4q\pi^2}{Ah} [C] |\langle S_C \rangle|^2 \frac{l_f}{(\frac{6}{\pi})^{1/3}} \frac{d_S^{-2/3}}{\sqrt{4\pi \lambda_S^N k_B T}} e^{-\frac{(\Delta V^0 + \lambda_S^N)^2}{4\lambda_S^N k_B T}} \quad \dots (13)$$

DOI:https://doi.org/10.25130/tjps.v31i4.2030

The atomic density d_S in semiconductor is function of nature concentration N_e at the Fermi level and Fermi energy E_F, and given by [16]:

$$d_S = \frac{3}{2D_n}\left(\frac{N_e}{E_F}\right) \quad \dots (14)$$

The fill factor for RuTh-TiO_2 solar cell is ratio relative to J_F-V curve's maximum power, it is a function of the maximum flow current density J_m and maximum voltage V_m, and gave by [17]:

$$FF = \frac{J_m V_m}{J_S V_o} \quad \dots (15)$$

where J_S and V_o are short-circuiting current and open circuit voltages. The efficiency of RuTh-TiO_2 solar cell can be written as [18]:

$$\eta\% = \frac{FF J_S V_o}{I_n} \quad \dots (16)$$

where I_n is incident light intensity.

RESULTS

The flow current $I_F(E)$ and current density $J_F(E)$ for charge transfer from RuTh dye to TiO_2 were calculated by using Eq.(12) together Eq.(13) by taken the reorganization energy λ_S^N (eV) in Eq.(6) ,the driving force energy ΔV^0, strength coupling $|\langle S_C \rangle|$,carrier concentration and atomic density of TiO_2 semiconductorl in Eq.(11) and Eq.(14) and effective path length l_f at room temperature ($k_B T = 0.025$eV).The physical characteristic of TiO_2 semiconductor lists in Table (1).

Table 1: Physical properties of TiO_2.

Properties	Quantity
Density	4.23(g/cm3) [19]
Atomic weight	79.866 (g/mol) [19]
Crystal structure	Tetragonal rutile[19]
Lattice constant (Å)	a=4.5936 c=2.9587[19]
Refractive index	2.609 [19]
Dielectric constant	55[20]
Radius Calculated (Å)	1.956
carrier concentration	$N_e = 1.4 \times 10^{14} (cm^{-3})$[20]
Fermi energy (E_F)	$4.52 eV$ [20]
effective density of states (D_n)	8 (state /eV) [20]

However, the reorganization energy λ_S^N (eV) for electron transfer in the RuTH-TiO_2 system has been evaluated according to estimate the radii of RuTh dye and TiO_2 semiconductor by using the Eq. (7) with inserting the molecule weight for RuTh is (1188.55 g/mol) and (79.866 g/mol) for TiO_2 and density for RuTh dye is (1.52 g/cm³) and (4.23 g/cm³) for TiO_2, the results calculation using approximated Eq. (7) are ($D_{RuTh} = 6.769$ Å) and ($D_{TiO_2} = 1.956 A^o$) for RuTh dye and TiO_2, respectively. The reorganization energy λ_S^N (eV) calculates using Eq.(6) of the RuTh-TiO_2 system with ethyl alcohol solvent in RuTh-TiO_2 DSSCs by insert dielectric constant (55) and refractive (2.609) of TiO_2 semiconductor from Table (1) and dielectric constant of ethyl alcohol solvent (24.5) and refractive (1.361) with [21] in Eq. (8) with to results ($\lambda_S^N = 0.404\ eV$). Another factor help to calculate the flow current is the atomic constant , it calculates used Eq. (14) by taken account ($N_e = 1.4 \times 10^{14} cm^{-3}$), ($E_F = 4.52\ eV$) and ($D_n = 8$ state/eV) of TiO_2 from Table (1) to result ($d_S = 5.8 \times 10^{18} m^{-3}$). The flow current $I_F(E)$ for RuTh dye to TiO_2 with ethyl alcohol solvent can calculate using Eq. (12) taken into account the coupling ($|\langle S_C \rangle|$ =0.38, 0.50, 0.59, 0.67, 0.74, 0.80, 0.86, 0.92, 0.97, 1.02, 1.07, 1.11, 1.16, 1.20, and 1.24×10^{-1} eV), ($\lambda_S^N = 0.404\ eV$), ($l_f = 3\ A^o$) [22], ($d_S = 5.8 \times 10^{18} (m^{-3})$), and taken two carrier concentration ($[C] = (2,4) \times 10^{18}\ cm^{-3}$) [23] using MATLAP program, results show in the Table (1). The flow current density $J_F(E)$ can calculate using Eq. (13) taking into account the results shown in Table (2) and the cell area ($0.49\ cm^2$) [24] to the list of results in Table (3).

DOI:https://doi.org/10.25130/tjps.v31i4.2030

Table 2: Results of flow current $I_F(A)$ for RuTH-$TiO_2$with ethyl alcohol solvent.

Strength coupling [22] $\lvert\langle S_C\rangle\rvert \times 10^{-1}$ (eV)	The flow current $I_F(A)$	
	Carrier concentration	
	$2 \times 10^{18}(cm^{-3})$	$4 \times 10^{18}(cm^{-3})$
0.38	0.917E-03	1.834E-03
0.50	1.529E-03	3.058E-03
0.59	2.141E-03	4.282E-03
0.67	2.752E-03	5.505E-03
0.74	3.364E-02	6.729E-03
0.80	3.976E-02	7.953E-03
0.86	4.588E-02	9.176E-03
0.92	5.200E-02	10.400E-03
0.97	5.812E-02	1.162E-02
1.02	6.424E-02	1.284E-02
1.07	7.033E-02	1.405E-02
1.11	7.646E-02	1.529E-02
1.16	8.253E-02	1.650E-02
1.20	8.866E-02	1.773E-02
1.24	9.480E-02	1.896E-02

Table 3: Results of flow current density $J_F(A/cm^2)$for RuTH-TiO_2 with ethyl alcohol solvent.

Strength coupling [22] $\lvert\langle S_C\rangle\rvert \times 10^{-1}$ (eV)	The flow current density $J_F(A/cm^2)$	
	Carrier concentration	
	$2 \times 10^{18}(cm^{-3})$	$4 \times 10^{18}(cm^{-3})$
0.38	1.736	3.473
0.50	3.121	6.242
0.59	3.009	6.018
0.67	5.618	11.236
0.74	6.866	13.733
0.80	8.115	16.230
0.86	9.364	18.727
0.92	10.612	21.225
0.97	11.861	23.722
1.02	13.11	26.22
1.07	14.358	28.717
1.11	15.606	31.213
1.16	16.855	33.710
1.20	18.104	36.209
1.24	19.353	38.706

Indeed, the photocurrent characteristics of RuTh-TiO_2 solar cell was limited by increasing concentration, coupling constant and flow current density. In contrast, the J_F-V results can be shown in Table (4). The characteristic of $J_F(E) - V$ curves of RuTH dye-contact with TiO_2 in solar cell devices using two concentrations (2×10^{18} cm-^{3}) and (4×10^{18} cm-^{3}) are shown in Figure (2).

DOI:https://doi.org/10.25130/tjps.v31i4.2030

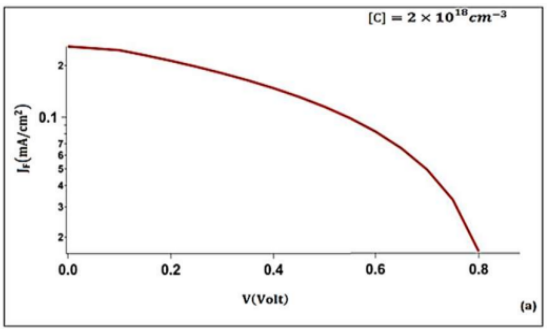
Table 4. The J_F-V characteristic of RuTH-TiO_2 devices.

Carrier concentration			
2×10^{18} (cm^{-3})		4×10^{18} (cm^{-3})	
V(Volt)	$J_F(\frac{mA}{cm^2})$	V(Volt)	$J_F(\frac{mA}{cm^2})$
0.81	0	0.82	0
0.80	1.736	0.8	3.473
0.75	3.121	0.75	6.242
0.7	3.009	0.7	6.018
0.65	5.618	0.65	11.236
0.6	6.866	0.6	13.733
0.55	8.115	0.55	16.230
0.5	9.364	0.5	18.727
0.45	10.612	0.45	21.225
0.4	11.861	0.4	23.722
0.35	13.11	0.35	26.22
0.3	14.358	0.3	28.717
0.25	15.606	0.25	31.213
0.2	16.855	0.2	33.710
0.15	18.104	0.15	36.209
0.1	19.353	0.1	38.706
0	20.624	0	40.19

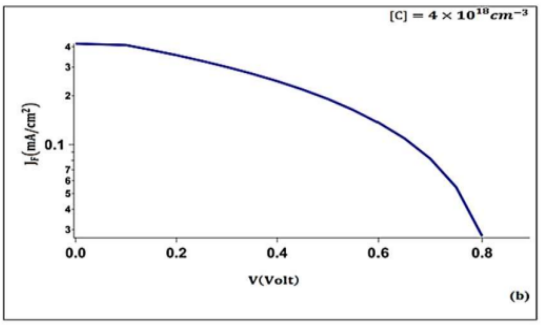
Filling factor and efficiency can be evaluated using Eq. (6) together Eq. (17), respectively using data in Table (4), as well as Figure (2), results list in the Table (5) for RuTH-TiO_2 devices.

Table 5. The J_{Sc} (mA/cm^2), V_{oc} (V), J_m (mA/cm^2), V_m (V), fill factor (FF) and efficiency of RuTH-TiO_2 DSSCs.

Variables	The electronic concentration	
	2 $\times 10^{18}(cm^{-3})$	**4** $\times 10^{18}(cm^{-3})$
J_{Sc}(mA/ cm^2)	20.624	40.19
V_{oc} (V)	0.81	0.82
J_m(mA/ cm^2)	11.325	22.423
V_m (V)	0.402	0.412
FF	0.272	0.280
Efficiency	4.543 %	9.227 %



(a)



(b)

Fig. 2: The flow current density versus voltage at: (a) 2×10^{18} (cm^{-3}), (b) 4×10^{18} (cm^{-3}).

DISCUSSION

In the results, the numerical data for calculating the reorganization energy λ_S^N (eV), flow current I_F(A) and charge transfer current density J_F (mA/cm^2) from the excited state in RuTh dye to the conduction band in TiO_2 are presented using charge transfer in the RuTH-TiO_2 system. This is calculated for different strength coupling in range ($(0.38\ eV \leq |\langle S_C \rangle| \leq 1.24\ \text{eV}) \times 10^{-1}$) at room temperature (300 K), with the inclusion of the effective density, atomic density and the driving energy, as well as two carrier concentration of TiO_2 semiconductor ($[C] = (2,4) \times 10^{18} cm^{-3}$), respectively. The reorganization energy is calculated using values of the optical and dielectric constants of ethyl alcohol solvent and TiO_2, which influenced the energy transport. In Table (2), we show the calculation of the flow current $I_F(A)$ under different strength coupling and carrier concentration at finite reorganization energy, which are critical parameters for the

charge transport process. These two parameters indicate the flow current $I_F(A)$ behavior of the RuTh-TiO_2 system. The evolution of flow current is shown in Table (2), where it observes that flow current increases with the strength coupling, with values ranging from (0.38 eV) to (1.24 eV), it reach to maximum (9.480E-03 A) with concentration ($2 \times 10^{18} cm^{-3}$) corresponding to flow current (1.896E-02 A) with concentration ($4 \times 10^{18} cm^{-3}$), respectively. Stronger electronic coupling enhances charge transfer rates, reduces recombination, and lowers resistance, leading to higher electronic transfer current in in the RuTH-TiO_2 system. By increasing the concentration of carrier, it directly enhance the exchange current and the limiting current, leading to higher electronic transfer currents. That indicated the flow charge increases with increases concentration and vice versa. Additionally, the flow charge increases as the strength coupling $|\langle S_C \rangle|$ of the system increases, with values starting from (9.17E-04 A) at ($|\langle S_C \rangle|$ =0.38×10^{-1} eV) to reach (9.480E-03 A) at ($|\langle S_C \rangle|$ =1.24×10^{-1} eV) with concentration ([c]= $2 \times 10^{18} cm^{-3}$)comparing from (1.834E-03 A) to (1.896E-02 A) at concentration ([c]= $4 \times 10^{18} cm^{-3}$). On the other hand, the flow current density $J_F \left(\frac{mA}{cm^2}\right)$ increases as the concentration increases, from (1.736) to (19.353) at ($[C] = 2 \times 10^{18} cm^{-3}$) comparing increases from (3.473) to (38.706) at ($[C] = 4 \times 10^{18} cm^{-3}$). However, it is observed that the flow current density $J_F \left(\frac{mA}{cm^2}\right)$ remains relatively increases and shows little variation with changes in strength coupling ranging from (0.38 eV) to (1.24 eV). The current density in RuTh-TiO_2 system generally increases with increasing concentration of the electroactive species, but the relationship depends on the reaction kinetics and mass transport conditions. The interactions between RuTh dye and TiO_2 atoms include force covalent bonds, and the driving force and reorganization energy of system plays a crucial role in electron transfer. Furthermore, the electronic transport occurred through the interface was affected under alignment of energy levels of two RuTh dye and TiO_2 materials with different strength coupling and is influenced by concentration and reorganization energy and band alignment. Furthermore, the calculated fill factor and efficiency in Table (5) shows a clear relationship with flow current density and concentration, as concentration energy increases, the efficiency increases, and vice versa. Specifically, as concentration carrier increases from ($2 \times 10^{18}\ cm^{-3}$) to ($4 \times 10^{18} cm^{-3}$) , the current density $J_{Sc}(mA/cm^2)$ values also increase from (20.624) to (40.19) and maximum flow current density $J_m(mA/cm^2)$ increases from (11.325) to (22.423). This suggests that as the efficiency increases from (4.543 %) to (9.227 %), the charge transport for from RuTH dye to TiO_2 semiconductors increases. However, the fill factor less increases with increase concentration from (0.272) to (0.280). The stability of RuTh-TiO_2 solar cell played an important role in electronic transport and strongest depending on the morphological as well as structural properties of RuTh and TiO_2 materials.

CONCLUSION

In conclusion, our flow current density, fill factor, as well as efficiency calculations show that flow current in RuTh-TiO_2 device influenced by the strength coupling and carrier concentration, enhances both the reorganization energy and the electronic transport in the RuTh-TiO_2 system. The overall calculation of the efficiency, as a function of reorganization energy, current density, driving energy, concentration, and coupling strength, yields to improve results for the electron transport process from RuTH dye to TiO_2 semiconductor. The consideration and strength coupling play a crucial role in the calculation of flow current density, particularly with high concentration and coupling strength. The electron transport current increases with increasing concentration and

strong coupling and reaches its maximum at equilibrium between mobility and transport. Thus, this donor-acceptor model provided more accurated and reliabled results comparing to other theoretical models used to investigation the mechanism of charge transport in the RuTH-TiO_2 system.

Conflict of interests: The authors declared no conflicting interests.

Sources of funding: This research didn't receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Author contribution: Authors contributed equally in the study.

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